Acta Crystallographica Section C
Structural Chemistry
ISSN 2053-2296

(5*RS*)-5-(4-Methoxyphenyl)-2-(methylsulfanyl)benzo[*g*]pyrimido[4,5-*b*]quinoline-4,6,11(3*H*,5*H*,12*H*)-trione, with Z' = 3, forms a three-dimensional hydrogen-bonded framework containing five types of hydrogen bond

Yelder A. Castillo,[a] Luis F. Zapata,[a] Jorge Trilleras,[a] Justo Cobo[b] and Christopher Glidewell[c]*

[a]Grupo de Investigación en Compuestos Heterocíclicos, Programa de Química, Facultad de Ciencias Básicas, Universidad del Atlántico, Barranquilla, Colombia, [b]Departamento de Química Inorgánica y Orgánica, Universidad de Jaén, 23071 Jaén, Spain, and [c]School of Chemistry, University of St Andrews, Fife KY16 9ST, Scotland
Correspondence e-mail: cg@st-andrews.ac.uk

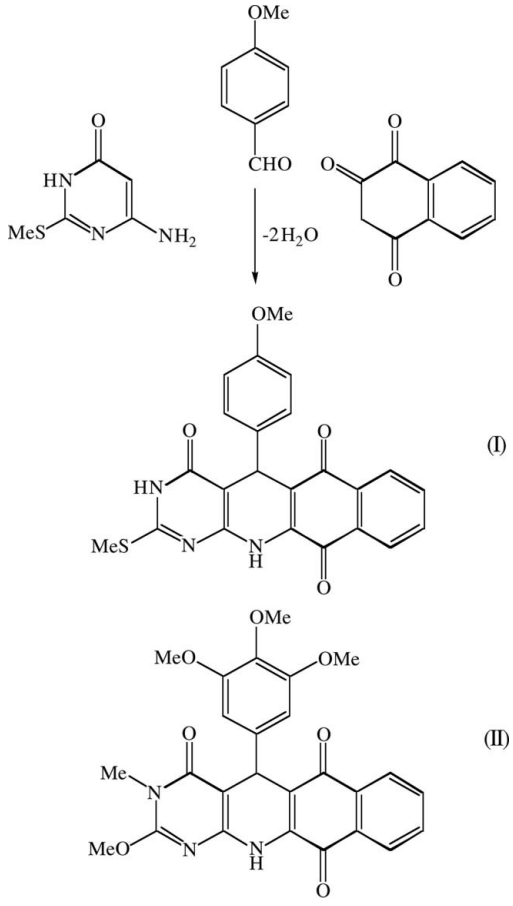
Received 5 November 2013
Accepted 4 December 2013

The title compound, $C_{23}H_{17}N_3O_4S$, crystallizes with Z' = 3 in the space group $P\overline{1}$. Two of the three independent molecules are broadly similar in terms of both their molecular conformations and their participation in hydrogen bonds, but the third molecule differs from the other two in both of these respects. The molecules are linked by a combination of N—H···O, N—H···N, C—H···O, C—H···N and C—H···π(arene) hydrogen bonds to form a continuous three-dimensional framework structure within which a centrosymmetric six-molecule aggregate can be identified as a key structural element.

Keywords: crystal structure; hydrogen bonding; supramolecular aggregation; six-molecule aggregate.

1. Introduction

Pyrimido[4,5-*b*]quinolines (also known as 5-deazaflavins) have been a focus of interest in medicinal chemistry because their biological properties, such as antimicrobial (El-Sayed *et al.*, 2002; Nadaraj *et al.*, 2012), antitumour (Alqasoumi *et al.*, 2010; El-Ashmawy *et al.*, 2013; El-Gohary, 2013) and analgesic activities (El-Gazzar *et al.*, 2008, 2009). As part of a program aimed at the development of new multicomponent reaction protocols we have now prepared the title benzo[*g*]pyrimido[4,5-*b*]quinoline-4,6,11(3*H*,5*H*,12*H*)-trione, (I) (Fig. 1), using a cyclocondensation reaction involving naphthalene-1,2,4(3*H*)-trione, an arylaldehyde and a 6-aminopyrimidine-4(3*H*)-one (see Scheme). The reaction was conducted under solvent-free conditions and was promoted by microwave irradiation. We report here the molecular and supramolecular structure of compound (I), which we compare briefly with that of 2-methoxy-3-methyl-5-(3,4,5-trimethoxyphenyl)benzo[*g*]-pyrimido[4,5-*b*]quinoline-4,6,11(3*H*,5*H*,12*H*)-trione, (II) (see Scheme), which had been prepared using an entirely analogous three-component condensation reaction (Castillo *et al.*, 2013).



2. Experimental

2.1. Synthesis and crystallization

An intimate mixture containing equimolar quantities of 6-amino-2-(methylsulfanyl)pyrimidin-4(3*H*)-one, naphthalene-1,2,4(3*H*)-trione and 4-methoxybenzaldehyde was subjected to microwave irradiation for 5 min at 300 W maximum power and 473 K in a CEM Discover microwave oven. Upon completion of the reaction, as monitored by thin-layer chromatography, the reaction mixture was cooled to ambient temperature. Recrystallization from ethanol, at ambient temperature and in air, provided yellow crystals suitable for single-crystal X-ray diffraction [yield 80%, m.p. > 573 K (decomposition)]. MS: (70 eV) m/z = 431 (61, M^+), 325 (19), 324 (100), 276 (18), 248 (12).

2.2. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. All H atoms were located in

  doi:10.1107/S2053229613032956

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{17}N_3O_4S$
M_r	431.47
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	120
a, b, c (Å)	11.020 (3), 12.138 (5), 23.139 (5)
α, β, γ (°)	85.33 (3), 79.56 (2), 74.33 (3)
V (Å^3)	2929.0 (16)
Z	6
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.20
Crystal size (mm)	0.40 × 0.27 × 0.10
Data collection	
Diffractometer	Bruker–Nonius KappaCCD diffractometer
Absorption correction	Multi-scan (*SADABS*; Sheldrick, 2003)
T_{min}, T_{max}	0.923, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	82441, 13434, 7678
R_{int}	0.091
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.650
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.068, 0.153, 1.02
No. of reflections	13434
No. of parameters	844
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.51, −0.38

Computer programs: *COLLECT* (Hooft, 1998), *DIRAX*/*LSQ* (Duisenberg *et al.*, 2000), *EVALCCD* (Duisenberg *et al.*, 2003), *SIR2004* (Burla *et al.*, 2005), *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

difference maps. H atoms bonded to C atoms were then treated as riding atoms in geometrically idealized positions, with C—H distances of 0.95 (aromatic), 0.98 (methyl) or 1.00 Å (aliphatic C—H) and with $U_{iso}(H) = kU_{eq}(C)$, where k = 1.5 for the methyl groups, which were permitted to rotate but no tot tilt, and 1.2 for all other H atoms bonded to C atoms. H atoms bonded to N atoms were permitted to ride at the positions located in difference maps, with $U_{iso}(H) = 1.2U_{eq}(N)$, giving the N—H distances shown in Table 2.

3. Results and discussion

Compound (I) crystallizes in the space group $P\overline{1}$ with $Z' = 3$; it will be convenient to refer to the molecules containing atoms N11, N21 and N31 (Fig. 1) as types 1, 2 and 3, respectively. Each molecule of compound (I) contains a stereogenic centre, at atoms C15, C25 and C35, respectively, but the centrosymmetric space group confirms that the compound crystallizes as a racemic mixture. By selecting the reference molecules of types 1 and 2 to have the *R* configuration at atoms C15 and C25, respectively, while the type 3 molecule has the *S* configuration at atom C35, it is possibly to assemble a compact asymmetric unit in which the three reference molecules are linked by four hydrogen bonds, two each of N—H···O and N—H···N types (Table 2), and it is to this selection of reference molecules that the deposited atomic coordinates and the derived geometrical parameters refer. However, the conformational parameters in Table 3 all refer to the *R* configura-

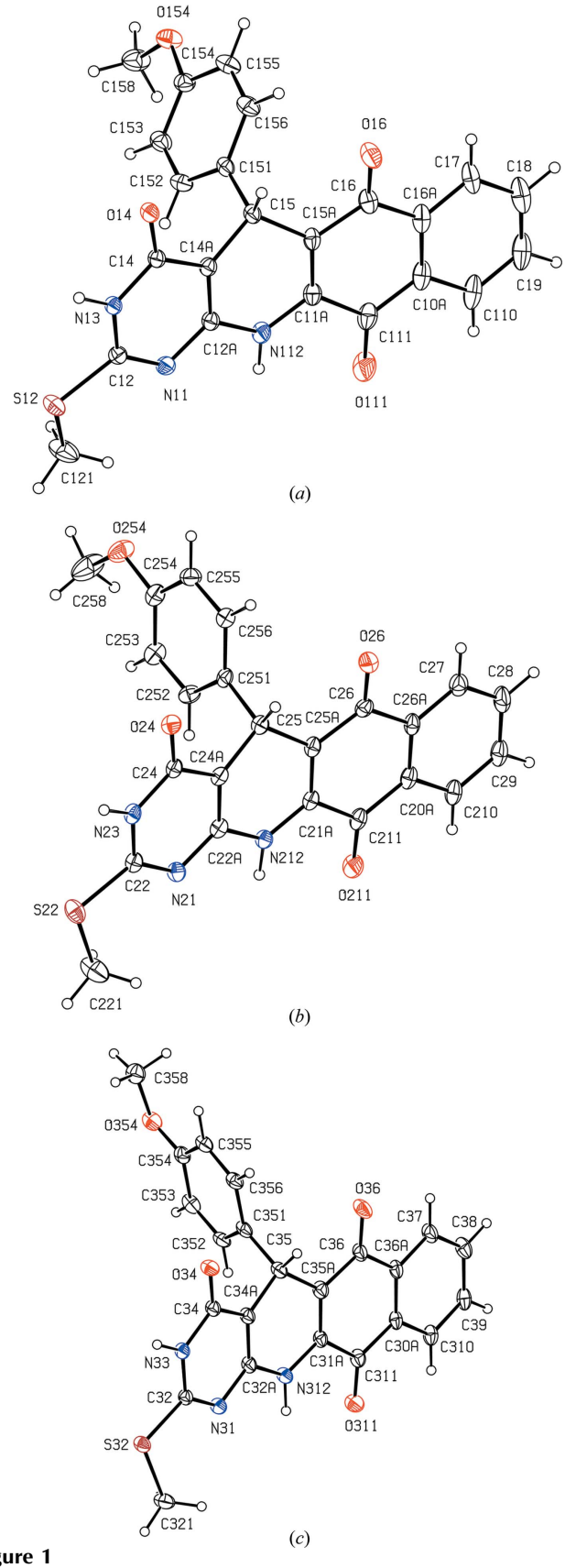


Figure 1
The *R* enantiomers of the three independent molecules of compound (I), showing the atom-labelling schemes for (*a*) a type 1 molecule, (*b*) a type 2 molecule and (*c*) a type 3 molecule. Displacement ellipsoids are drawn at the 30% probability level.

Table 2
Hydrogen-bond geometry (Å, °).

Cg represents the centroid of the C251–C256 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N13—H13···O34	0.92	1.84	2.757 (3)	173
N23—H23···O24^{i}	0.93	1.81	2.741 (3)	176
N33—H33···O14	0.87	1.86	2.702 (3)	160
N112—H112···N21	0.95	2.28	3.175 (4)	156
N212—H212···N11	0.98	2.21	3.125 (4)	154
C255—H255···O26^{ii}	0.95	2.34	3.237 (4)	158
C352—H352···N31^{iii}	0.95	2.61	3.503 (4)	157
C29—H29···*Cg*^{iv}	0.95	2.79	3.659 (4)	152

Symmetry codes: (i) $-x, -y+1, -z$; (ii) $-x+1, -y, -z$; (iii) $-x+2, -y+1, -z+1$; (iv) $x+1, y, z$.

tions of the three independent molecules and the three molecule shown in Fig. 1 are the three *R* enantiomers.

Within this asymmetric unit, molecules of types 1 and 2 are linked by pairs of N—H···N hydrogen bonds in an $R_2^2(8)$ (Bernstein *et al.*, 1995) motif, while molecules of types 1 and 3 are linked by pairs of N—H···O hydrogen bonds to form a second $R_2^2(8)$ motif.

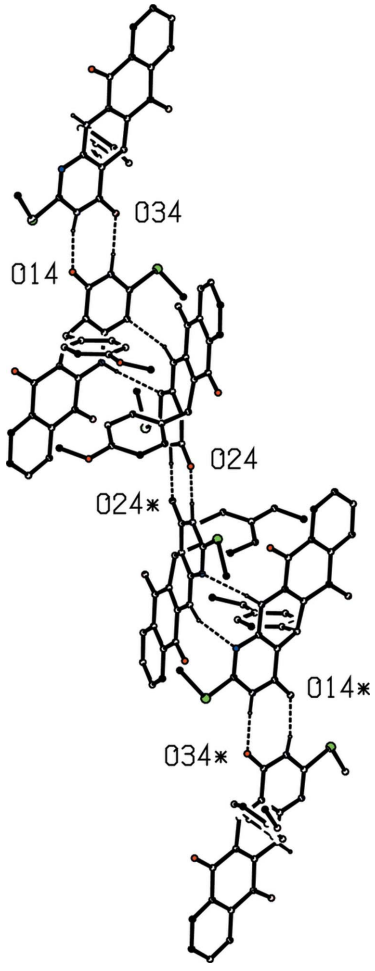


Figure 2
Part of the crystal structure of compound (I), showing the formation of a centrosymmetric six-molecule aggregate containing ten hydrogen bonds. For the sake of clarity, H atoms bonded to C atoms have been omitted, as has the unit-cell outline. Atoms marked with an asterisk are at the symmetry position $(-x, -y+1, -z)$.

Table 3
Selected geometric parameters (Å, °) for the *R* enantiomers of the three independent molecules in compound (I).

Ring-puckering angles are defined for the atom sequences N*x*12—C*x*1*A*—C*x*5*A*—C*x*5—C*x*4*A*—C*x*2*A* for $x = 1$, 2 or 3.

(*a*) Torsion and bond angles	Molecule 1 $x = 1$	Molecule 2 $x = 2$	Molecule 3 $x = 3$
N*x*1—C*x*2—S*x*2—C*x*21	−16.4 (3)	3.1 (3)	8.6 (3)
C*x*4*A*—C*x*5—C*x*51—C*x*52	−15.5 (4)	−48.0 (4)	−71.1 (3)
C*x*5*A*—C*x*5—C*x*51—C*x*52	94.5 (3)	72.4 (4)	50.3 (4)
C*x*53—C*x*54—O*x*54—C*x*58	−12.7 (5)	−6.1 (5)	171.0 (3)
N*x*1—C*x*2—S*x*2	122.2 (2)	122.3 (3)	122.6 (2)
N*x*3—C*x*2—S*x*2	114.3 (2)	114.1 (2)	114.0 (2)
C*x*53—C*x*54—O*x*54	124.5 (3)	124.0 (3)	116.4 (3)
C*x*55—C*x*54—O*x*54	116.0 (3)	115.7 (3)	124.5 (3)

(*b*) Ring-puckering parameters	Molecule 1	Molecule 2	Molecule 3
Q	0.246 (4)	0.185 (4)	0.120 (4)
θ	111.4 (9)	113.8 (9)	109.5 (19)
φ	4.9 (9)	10.2 (12)	8.4 (19)

For the *R* enantiomer of each of the independent molecules, the ring-puckering parameters (Cremer & Pople, 1975) show (Table 3) that the rings containing atoms N*x*1 (where $x = 1$, 2 or 3) adopt conformations fairly close to boat forms for which the idealized values of the puckering angles are $\theta = 90°$ and $\varphi = 60k°$, where *k* represents an integer. The orientations of the methylsulfanyl units relative to the adjacent pyrimidine rings are all fairly similar, as are the orientations of the pendent aryl rings relative to the adjacent reduced pyridine rings, but the values of the torsion angles C*x*4*A*—C*x*5—C*x*51—C*x*52 and C*x*5*A*—C*x*5—C*x*51—C*x*52 differ sufficiently among the three independent molecules effectively to preclude the possibility of any additional crystallographic symmetry.

However, the principal conformational difference between the molecules, which definitively rules out the possibility of any additional symmetry, is the orientation of the methoxy substituent. In the molecules of types 1 and 2, the methyl C*x*58 atoms are fairly close to the plane of the adjacent aryl rings, displaced by 0.381 (4) and 0.047 (6) Å, respectively, and oriented away from the C*x*5—H*x*5 bond, but in the type 3 molecule, where the methyl C atom is displaced from the adjacent ring plane by 0.169 (4) Å, the methoxy substituent is oriented towards the C35—H35 bond (Fig. 1 and Table 3).

In each of the molecules, the two exocyclic C—C—O angles at the C*x*54 atoms differ by around 10° (Table 3), as is often found in methoxyphenyl units in which the methyl C atom is effectively coplanar with the adjacent ring (Seip & Seip, 1973; Ferguson *et al.*, 1996; Patterson *et al.*, 1998). An exactly comparable pattern is observed for the exocyclic N—C—S angles at atoms C12, C22 and C32 (Table 3).

The hydrogen bonds formed by the type 3 molecule differ from those formed by the molecules of types 1 and 2 (Table 2). In particular, the type 3 molecule forms no N—H···N hydrogen bonds and, indeed, the N312—H312 bond plays no role in the supramolecular assembly, forming only a short intramolecular contact with an N—H···O angle of only 102°, which is far too small for this contact to be significant (*cf.* Wood *et al.*, 2009). In addition, where the N11 and N21 atoms

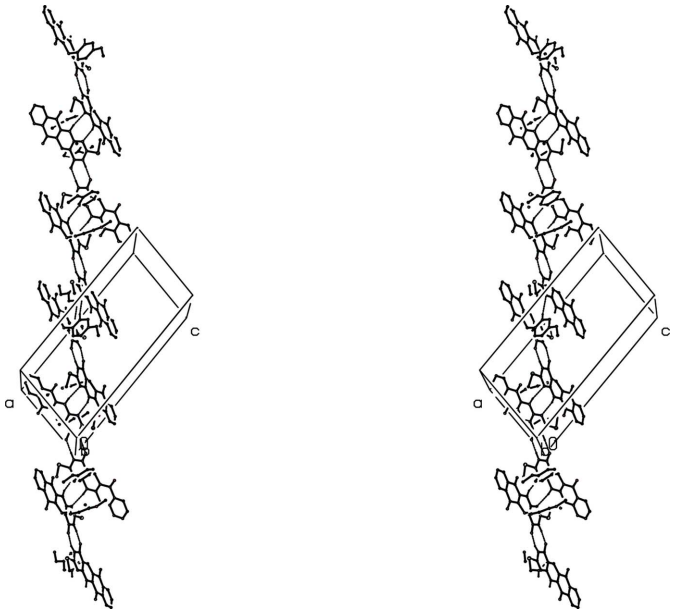


Figure 3
A stereoview of part of the crystal structure of compound (I), showing the formation of a chain of rings along [201] built from N—H···O, N—H···N and C—H···N hydrogen bonds. For the sake of clarity, H atoms bonded to C atoms but not involved in the motifs shown have been omitted.

act as acceptors in N—H···N hydrogen bonds, the N31 atom acts as an acceptor only in a C—H···N hydrogen bond, where the H···N distance (Table 2) is well below the sum, 2.75 Å, of the van der Waals radii (Bondi, 1964; Rowland & Taylor, 1996). Thus, while the molecules of types 1 and 2 are broadly similar, both in their molecular conformations and in their hydrogen-bonding characteristics, at least so far as the N—H···O and N—H···N interactions are concerned, the type 3 molecule shows significant differences from the other two in both of these respects. There are no short intermolecular contacts involving the S atoms; in any event, it is well established that two-connected S atoms of the type found here are extremely poor hydrogen-bond acceptors (Allen *et al.*, 1997). In this connection, it is worth noting here that the O atom of the corresponding methoxy group in compound (II) (see Scheme; Castillo *et al.*, 2013) likewise does not act as an acceptor of hydrogen bonds. Similarly, none of the methoxy groups in the three independent 4-methoxyphenyl groups in (I) or in the 3,4,5-trimethoxyphenyl group of (II) accept any hydrogen bonds. It is thus not surprising that the S atom in (I) plays no role in the supramolecular assembly.

As noted above, four hydrogen bonds link the three independent molecules in the selected asymmetric unit and, in addition, an inversion-related pair of N—H···O hydrogen bonds links two of these three-molecule units to form a centrosymmetric six-molecule aggregate containing a total of ten hydrogen bonds, six of N—H···O type and four of N—H···N type, arranged into five $R_2^2(8)$ rings, three built from pairs of N—H···O hydrogen bonds and two from pairs of N—H···N hydrogen bonds (Fig. 2). Three further hydrogen bonds, one each of C—H···N, C—H···O and C—H···π(arene) types link the six-molecule aggregates into a continuous three-dimensional framework structure, whose formation is readily analysed in terms of three one-dimensional substructures (Ferguson *et al.*, 1998*a*,*b*; Gregson *et al.*, 2000), each utilizing just one of these three further hydrogen bonds. The six-molecule aggregate identified above forms a convenient basis for the descriptive analysis of the supramolecular assembly; since, however, the overall assembly is a continuous three-dimensional array, this six-molecule aggregate has no special structural significance beyond its utility for the purpose of simplifying the description.

The six-molecule aggregates are linked by the C—H···N hydrogen bond to form a chain of rings running parallel to the [201] direction, where inversion-related pairs of C—H···N hydrogen bonds generate $R_2^2(14)$ motifs (Fig. 3). The C—H···O hydrogen bond, on the other hand, links the aggregates into a second chain of rings, now running parallel to the [1$\bar{1}$0] direction, and containing only $R_2^2(8)$ rings (Fig. 4); the chain construction requires only the participation of the type 1 and 2 molecules, with the type 3 molecules simply pendent from the chain itself. Finally, the C—H···π(arene) hydrogen bond generates a third chain of rings running parallel to the [100] direction, built from type 2 molecules only, with molecules of both types 1 and 3 pendent from it; here $R_2^2(8)$ rings containing inversion-related pairs of N—H···O hydrogen bonds and centred at (n, $\frac{1}{2}$, 0) alternate with larger rings built from inversion-related pairs of C—H···π(arene) hydrogen bonds and centred at ($n + \frac{1}{2}$, $\frac{1}{2}$, 0), where n represents an integer in each case (Fig. 5). Thus, the participation of the three independent molecules differs between each of these chains. The combination of these one-dimensional substructures running along [100], [1$\bar{1}$0] and [201] links all of the aggregates into a single three-dimensional structure.

It is of interest briefly to compare the structural properties of compound (I) with those of the analogous compound (II) (Castillo *et al.*, 2013). Compound (II) crystallizes in the space group $P\bar{1}$ as a partial hydrate having $Z' = 1$, and the components are linked by a combination of N—H···O and C—H···O hydrogen bonds to form a chain of rings; hence, in (II), with $Z' = 1$, the supramolecular aggregation is one-dimensional, whereas in (I), with $Z' = 3$, the supramolecular aggregation is three-dimensional.

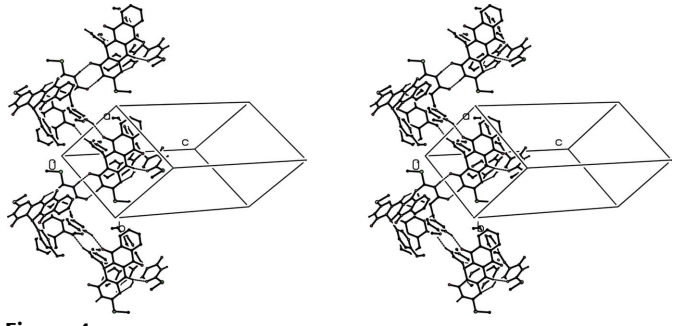


Figure 4
A stereoview of part of the crystal structure of compound (I), showing the formation of a chain of rings along [1$\bar{1}$0] built from N—H···O, N—H···N and C—H···O hydrogen bonds. For the sake of clarity, molecules of type 3 and H atoms bonded to C atoms but not involved in the motifs shown have been omitted.

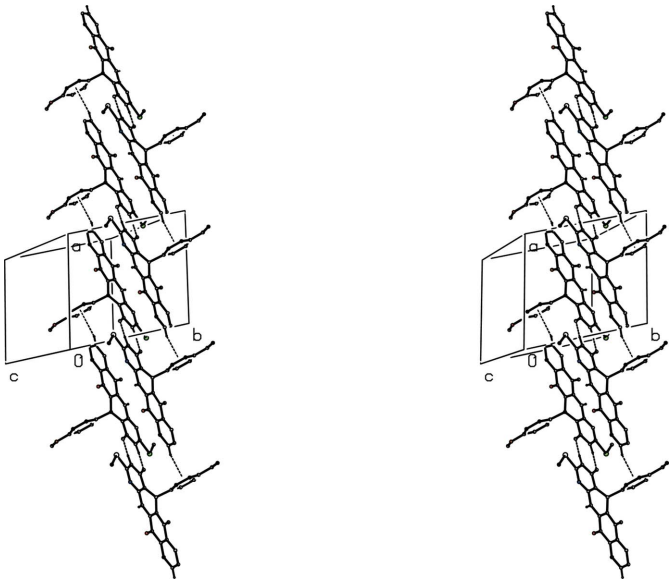


Figure 5
A stereoview of part of the crystal structure of compound (I), showing the formation of a chain of rings along [100] built from N—H···O and C—H···π(arene) hydrogen bonds. For the sake of clarity, molecules of types 1 and 3, and H atoms bonded to C atoms but not involved in the motifs shown have been omitted.

The authors thank 'Centro de Instrumentación Científico-Técnica of Universidad de Jaén' and the staff for data collection. YAC, LFZ and JT thank the Universidad del Atlántico and 'Fundación para la Promoción de la Investigación y la Tecnología – Banco de la República' Proyecto No. 2.627, Convenio No. 201001, for financial support. JC thanks the Consejería de Innovación, Ciencia y Empresa (Junta de Andalucía, Spain) and the Universidad de Jaén for financial support.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: YF3052). Services for accessing these data are described at the back of the journal.

References

Allen, F. H., Bird, C. M., Rowland, R. S. & Raithby, P. R. (1997). *Acta Cryst.* B**53**, 696–701.

Alqasoumi, S. I., Al-Taweel, A. M., Alafeefy, A. M., Noaman, E. & Ghorab, M. M. (2010). *Eur. J. Med. Chem.* **45**, 738–744.

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.

Bondi, A. (1964). *J. Phys. Chem.* **68**, 441–451.

Burla, M. C., Caliandro, R., Camalli, M., Carrozzini, B., Cascarano, G. L., De Caro, L., Giacovazzo, C., Polidori, G. & Spagna, R. (2005). *J. Appl. Cryst.* **38**, 381–388.

Castillo, Y. A., Zapata, L. F., Trilleras, J., Cobo, J. & Glidewell, C. (2013). Private communication (accession number 967598). CCDC, Cambridge, England.

Cremer, D. & Pople, J. A. (1975). *J. Am. Chem. Soc.* **97**, 1354–1358.

Duisenberg, A. J. M., Hooft, R. W. W., Schreurs, A. M. M. & Kroon, J. (2000). *J. Appl. Cryst.* **33**, 893–898.

Duisenberg, A. J. M., Kroon-Batenburg, L. M. J. & Schreurs, A. M. M. (2003). *J. Appl. Cryst.* **36**, 220–229.

El-Ashmawy, M. B., El-Sherbeny, M. A. & El-Gohary, N. S. (2013). *Med. Chem. Res.* **22**, 2724–2736.

El-Gazzar, A. B. A., El-Enany, M. M. & Mahmoud, M. N. (2008). *Bioorg. Med. Chem.* **16**, 3261–3273.

El-Gazzar, A. B. A., Hafez, H. N. & Nawwar, G. A. M. (2009). *Eur. J. Med. Chem.* **44**, 1427–1436.

El-Gohary, N. S. (2013). *Med. Chem. Res.* **22**, 5236–5247.

El-Sayed, O. A., Al-Bassam, B. A. & Hussein, M. E. (2002). *Arch. Pharm.* **335**, 403–410.

Ferguson, G., Glidewell, C., Gregson, R. M. & Meehan, P. R. (1998*a*). *Acta Cryst.* B**54**, 129–138.

Ferguson, G., Glidewell, C., Gregson, R. M. & Meehan, P. R. (1998*b*). *Acta Cryst.* B**54**, 139–150.

Ferguson, G., Glidewell, C. & Patterson, I. L. J. (1996). *Acta Cryst.* C**52**, 420–423.

Gregson, R. M., Glidewell, C., Ferguson, G. & Lough, A. J. (2000). *Acta Cryst.* B**56**, 39–57.

Hooft, R. W. W. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.

Nadaraj, V., Selvi, S., Mohan, S. & Thangadurai, T. (2012). *Med. Chem. Res.* **21**, 2911–2919.

Patterson, I. L. J., Glidewell, C. & Ferguson, G. (1998). *Acta Cryst.* C**54**, 1970–1974.

Rowland, R. S. & Taylor, R. (1996). *J. Phys. Chem.* **100**, 7384–7391.

Seip, H. M. & Seip, R. (1973). *Acta Chem. Scand.* **27**, 4024–4027.

Sheldrick, G. M. (2003). *SADABS*. University of Göttingen, Germany.

Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.

Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

Wood, P. A., Allen, F. H. & Pidcock, E. (2009). *CrystEngComm*, **11**, 1563–1571.

supplementary materials

Acta Cryst. (2014). C**70**, 50-54 [doi:10.1107/S2053229613032956]

(5*RS*)-5-(4-Methoxyphenyl)-2-(methylsulfanyl)benzo[*g*]pyrimido[4,5-*b*]quinoline-4,6,11(3*H*,5*H*,12*H*)-trione, with *Z*′ = 3, forms a three-dimensional hydrogen-bonded framework containing five types of hydrogen bond

Yelder A. Castillo, Luis F. Zapata, Jorge Trilleras, Justo Cobo and Christopher Glidewell

Computing details

Data collection: *COLLECT* (Hooft, 1998); cell refinement: *DIRAX/LSQ* (Duisenberg *et al.*, 2000); data reduction: *EVALCCD* (Duisenberg *et al.*, 2003); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

(5*RS*)-5-(4-Methoxyphenyl)-2-(methylsulfanyl)benzo[*g*]pyrimido[4,5-*b*]quinoline-4,6,11(3*H*,5*H*,12*H*)-trione

Crystal data

$C_{23}H_{17}N_3O_4S$
$M_r = 431.47$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 11.020$ (3) Å
$b = 12.138$ (5) Å
$c = 23.139$ (5) Å
$\alpha = 85.33$ (3)°
$\beta = 79.56$ (2)°
$\gamma = 74.33$ (3)°
$V = 2929.0$ (16) Å^3
$Z = 6$
$F(000) = 1344$
$D_x = 1.468$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 13434 reflections
$\theta = 2.5$–27.5°
$\mu = 0.20$ mm^{-1}
$T = 120$ K
Plate, colourless
0.40 × 0.27 × 0.10 mm

Data collection

Bruker-Nonius KappaCCD diffractometer
Radiation source: Bruker–Nonius FR591 rotating anode
Graphite monochromator
Detector resolution: 9.091 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
$T_{min} = 0.923$, $T_{max} = 0.980$
82441 measured reflections
13434 independent reflections
7678 reflections with $I > 2\sigma(I)$
$R_{int} = 0.091$
$\theta_{max} = 27.5°$, $\theta_{min} = 2.5°$
$h = -14\rightarrow14$
$k = -15\rightarrow15$
$l = -30\rightarrow30$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.068$
$wR(F^2) = 0.153$
$S = 1.02$
13434 reflections
844 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 3.7271P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} = 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.51$ e Å^{-3}
	$\Delta\rho_{min} = -0.38$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
N11	0.3978 (2)	0.5957 (2)	0.22925 (12)	0.0302 (6)
C12	0.4994 (3)	0.6106 (3)	0.24674 (13)	0.0264 (7)
N13	0.5594 (2)	0.5423 (2)	0.28768 (11)	0.0255 (6)
H13	0.6319	0.5519	0.2985	0.031*
C14	0.5252 (3)	0.4451 (3)	0.31220 (14)	0.0266 (7)
O14	0.5859 (2)	0.38237 (19)	0.34824 (10)	0.0324 (5)
C14A	0.4190 (3)	0.4233 (3)	0.29272 (14)	0.0264 (7)
C15	0.3876 (3)	0.3096 (3)	0.30818 (14)	0.0282 (7)
H15	0.3955	0.2881	0.3502	0.034*
C15A	0.2515 (3)	0.3209 (3)	0.29969 (14)	0.0307 (7)
C16	0.1854 (3)	0.2360 (3)	0.32839 (15)	0.0371 (8)
O16	0.2281 (2)	0.1701 (2)	0.36763 (11)	0.0470 (7)
C16A	0.0672 (3)	0.2294 (3)	0.30777 (15)	0.0404 (9)
C17	0.0154 (4)	0.1378 (4)	0.32732 (17)	0.0507 (11)
H17	0.0541	0.0800	0.3534	0.061*
C18	−0.0965 (4)	0.1333 (4)	0.3072 (2)	0.0637 (13)
H18	−0.1322	0.0705	0.3192	0.076*
C19	−0.1551 (4)	0.2178 (5)	0.27050 (19)	0.0621 (13)
H19	−0.2313	0.2134	0.2582	0.075*
C110	−0.1041 (3)	0.3092 (4)	0.25142 (17)	0.0523 (11)
H110	−0.1452	0.3679	0.2264	0.063*
C10A	0.0090 (3)	0.3143 (3)	0.26938 (15)	0.0417 (9)
C111	0.0689 (3)	0.4070 (3)	0.24610 (16)	0.0421 (9)
O111	0.0235 (3)	0.4834 (3)	0.21167 (13)	0.0624 (8)
C11A	0.1945 (3)	0.4033 (3)	0.26256 (14)	0.0316 (8)
N112	0.2508 (2)	0.4878 (2)	0.23656 (12)	0.0341 (7)
H112	0.2183	0.5402	0.2066	0.041*
C12A	0.3588 (3)	0.5019 (3)	0.25412 (14)	0.0274 (7)
S12	0.56759 (9)	0.72241 (7)	0.21852 (4)	0.0363 (2)
C121	0.4984 (4)	0.7670 (4)	0.15328 (18)	0.0596 (12)
H12A	0.5410	0.7121	0.1224	0.089*
H12B	0.5094	0.8429	0.1399	0.089*
H12C	0.4071	0.7704	0.1618	0.089*
C151	0.4765 (3)	0.2155 (3)	0.26919 (14)	0.0279 (7)
C152	0.5365 (3)	0.2385 (3)	0.21367 (15)	0.0334 (8)
H152	0.5282	0.3161	0.2006	0.040*
C153	0.6088 (3)	0.1524 (3)	0.17604 (15)	0.0367 (8)
H153	0.6492	0.1714	0.1381	0.044*
C154	0.6216 (3)	0.0398 (3)	0.19395 (15)	0.0329 (8)
C155	0.5643 (4)	0.0133 (3)	0.25010 (16)	0.0406 (9)
H155	0.5748	−0.0644	0.2632	0.049*

C156	0.4926 (3)	0.0995 (3)	0.28665 (15)	0.0373 (8)
H156	0.4530	0.0802	0.3247	0.045*
O154	0.6864 (2)	−0.0515 (2)	0.15964 (10)	0.0423 (6)
C158	0.7206 (4)	−0.0270 (3)	0.09858 (16)	0.0513 (10)
H18A	0.6457	0.0218	0.0835	0.077*
H18B	0.7509	−0.0987	0.0775	0.077*
H18C	0.7886	0.0127	0.0928	0.077*
N21	0.2029 (2)	0.6058 (2)	0.11220 (12)	0.0290 (6)
C22	0.0923 (3)	0.6184 (3)	0.09535 (14)	0.0286 (7)
N23	0.0746 (2)	0.5551 (2)	0.05314 (11)	0.0276 (6)
H23	−0.0032	0.5706	0.0396	0.033*
C24	0.1707 (3)	0.4670 (3)	0.02623 (14)	0.0257 (7)
O24	0.1509 (2)	0.41057 (18)	−0.01164 (10)	0.0310 (5)
C24A	0.2916 (3)	0.4477 (3)	0.04575 (13)	0.0253 (7)
C25	0.3946 (3)	0.3419 (3)	0.02720 (14)	0.0266 (7)
H25	0.4021	0.3330	−0.0160	0.032*
C25A	0.5211 (3)	0.3522 (3)	0.04039 (14)	0.0268 (7)
C26	0.6378 (3)	0.2731 (3)	0.01293 (14)	0.0288 (7)
O26	0.6356 (2)	0.2103 (2)	−0.02530 (11)	0.0393 (6)
C26A	0.7609 (3)	0.2692 (3)	0.03281 (14)	0.0299 (7)
C27	0.8711 (3)	0.1864 (3)	0.01159 (16)	0.0379 (8)
H27	0.8691	0.1340	−0.0163	0.045*
C28	0.9848 (3)	0.1809 (3)	0.03171 (18)	0.0447 (10)
H28	1.0602	0.1240	0.0176	0.054*
C29	0.9883 (3)	0.2575 (3)	0.07180 (17)	0.0412 (9)
H29	1.0663	0.2531	0.0850	0.049*
C210	0.8802 (3)	0.3400 (3)	0.09291 (15)	0.0356 (8)
H210	0.8835	0.3931	0.1202	0.043*
C20A	0.7645 (3)	0.3451 (3)	0.07387 (14)	0.0311 (8)
C211	0.6468 (3)	0.4312 (3)	0.09814 (15)	0.0312 (8)
O211	0.6444 (2)	0.4987 (2)	0.13469 (12)	0.0461 (7)
C21A	0.5255 (3)	0.4298 (3)	0.07841 (14)	0.0266 (7)
N212	0.4181 (2)	0.5088 (2)	0.10348 (11)	0.0270 (6)
H212	0.4184	0.5564	0.1357	0.032*
C22A	0.3011 (3)	0.5202 (3)	0.08592 (13)	0.0264 (7)
S22	−0.04467 (8)	0.71910 (8)	0.12509 (4)	0.0410 (2)
C221	0.0176 (4)	0.7892 (4)	0.17366 (19)	0.0607 (12)
H22A	0.0443	0.7359	0.2059	0.091*
H22B	−0.0488	0.8560	0.1897	0.091*
H22C	0.0912	0.8139	0.1519	0.091*
C251	0.3593 (3)	0.2378 (3)	0.06053 (14)	0.0268 (7)
C252	0.3190 (3)	0.2395 (3)	0.12117 (14)	0.0323 (8)
H252	0.3177	0.3048	0.1416	0.039*
C253	0.2810 (3)	0.1494 (3)	0.15261 (15)	0.0357 (8)
H253	0.2541	0.1526	0.1940	0.043*
C254	0.2826 (3)	0.0551 (3)	0.12310 (16)	0.0362 (8)
C255	0.3243 (3)	0.0498 (3)	0.06293 (15)	0.0358 (8)
H255	0.3261	−0.0159	0.0428	0.043*
C256	0.3636 (3)	0.1402 (3)	0.03213 (15)	0.0332 (8)

H256	0.3938	0.1354	−0.0090	0.040*
O254	0.2426 (3)	−0.0375 (2)	0.14941 (11)	0.0496 (7)
C258	0.2091 (5)	−0.0391 (4)	0.21191 (18)	0.0749 (15)
H28A	0.2781	−0.0249	0.2292	0.112*
H28B	0.1959	−0.1140	0.2260	0.112*
H28C	0.1301	0.0207	0.2235	0.112*
N31	0.9511 (2)	0.3615 (2)	0.44169 (11)	0.0282 (6)
C32	0.8469 (3)	0.3521 (3)	0.42515 (14)	0.0261 (7)
N33	0.7837 (2)	0.4275 (2)	0.38721 (11)	0.0276 (6)
H33	0.7088	0.4246	0.3808	0.033*
C34	0.8226 (3)	0.5229 (3)	0.36264 (14)	0.0283 (7)
O34	0.7645 (2)	0.58546 (19)	0.32588 (10)	0.0340 (5)
C34A	0.9324 (3)	0.5390 (3)	0.38219 (14)	0.0284 (7)
C35	0.9754 (3)	0.6465 (3)	0.36203 (15)	0.0314 (8)
H35	0.9812	0.6559	0.3184	0.038*
C35A	1.1076 (3)	0.6330 (3)	0.37730 (14)	0.0319 (8)
C36	1.1734 (3)	0.7219 (3)	0.35460 (15)	0.0327 (8)
O36	1.1301 (2)	0.7964 (2)	0.31947 (11)	0.0470 (7)
C36A	1.2949 (3)	0.7184 (3)	0.37640 (14)	0.0305 (7)
C37	1.3520 (3)	0.8078 (3)	0.36069 (16)	0.0389 (9)
H37	1.3143	0.8700	0.3365	0.047*
C38	1.4638 (3)	0.8063 (3)	0.38035 (16)	0.0395 (9)
H38	1.5023	0.8678	0.3697	0.047*
C39	1.5201 (3)	0.7158 (3)	0.41539 (15)	0.0356 (8)
H39	1.5973	0.7153	0.4284	0.043*
C310	1.4644 (3)	0.6265 (3)	0.43147 (14)	0.0332 (8)
H310	1.5034	0.5639	0.4551	0.040*
C30A	1.3500 (3)	0.6287 (3)	0.41264 (14)	0.0288 (7)
C311	1.2860 (3)	0.5365 (3)	0.43244 (14)	0.0313 (8)
O311	1.3267 (2)	0.4561 (2)	0.46526 (11)	0.0422 (6)
C31A	1.1609 (3)	0.5466 (3)	0.41238 (14)	0.0269 (7)
N312	1.1040 (2)	0.4617 (2)	0.43530 (11)	0.0297 (6)
H312	1.1478	0.4021	0.4627	0.036*
C32A	0.9916 (3)	0.4556 (3)	0.41895 (14)	0.0273 (7)
S32	0.77743 (8)	0.23980 (7)	0.44995 (4)	0.0312 (2)
C321	0.8967 (3)	0.1482 (3)	0.48793 (17)	0.0422 (9)
H32A	0.9789	0.1297	0.4613	0.063*
H32B	0.8720	0.0775	0.5013	0.063*
H32C	0.9046	0.1873	0.5219	0.063*
C351	0.8797 (3)	0.7529 (3)	0.39029 (14)	0.0307 (8)
C352	0.8693 (3)	0.7702 (3)	0.44935 (15)	0.0330 (8)
H352	0.9210	0.7148	0.4723	0.040*
C353	0.7866 (3)	0.8650 (3)	0.47587 (15)	0.0358 (8)
H353	0.7809	0.8744	0.5167	0.043*
C354	0.7102 (3)	0.9482 (3)	0.44258 (15)	0.0324 (8)
C355	0.7192 (3)	0.9324 (3)	0.38339 (15)	0.0328 (8)
H355	0.6681	0.9880	0.3603	0.039*
C356	0.8027 (3)	0.8354 (3)	0.35774 (15)	0.0330 (8)
H356	0.8076	0.8249	0.3171	0.040*

O354	0.6322 (2)	1.0414 (2)	0.47199 (10)	0.0404 (6)
C358	0.5388 (3)	1.1202 (3)	0.44166 (17)	0.0433 (9)
H38A	0.5826	1.1529	0.4065	0.065*
H38B	0.4885	1.1817	0.4678	0.065*
H38C	0.4820	1.0793	0.4301	0.065*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N11	0.0287 (14)	0.0292 (15)	0.0350 (16)	−0.0082 (12)	−0.0122 (12)	0.0029 (12)
C12	0.0274 (17)	0.0251 (17)	0.0276 (17)	−0.0072 (13)	−0.0055 (14)	−0.0031 (13)
N13	0.0248 (13)	0.0271 (14)	0.0288 (14)	−0.0106 (11)	−0.0113 (11)	0.0025 (11)
C14	0.0249 (16)	0.0267 (17)	0.0313 (18)	−0.0095 (13)	−0.0096 (14)	0.0009 (14)
O14	0.0299 (12)	0.0336 (13)	0.0412 (14)	−0.0152 (10)	−0.0196 (11)	0.0092 (10)
C14A	0.0243 (16)	0.0287 (17)	0.0288 (17)	−0.0090 (13)	−0.0078 (14)	−0.0001 (14)
C15	0.0269 (16)	0.0315 (18)	0.0320 (18)	−0.0136 (14)	−0.0131 (14)	0.0052 (14)
C15A	0.0266 (17)	0.041 (2)	0.0282 (18)	−0.0154 (15)	−0.0056 (14)	0.0003 (15)
C16	0.039 (2)	0.045 (2)	0.032 (2)	−0.0202 (17)	−0.0031 (16)	−0.0040 (17)
O16	0.0498 (16)	0.0530 (17)	0.0456 (16)	−0.0278 (13)	−0.0102 (13)	0.0108 (13)
C16A	0.035 (2)	0.061 (3)	0.032 (2)	−0.0250 (18)	0.0021 (16)	−0.0126 (18)
C17	0.049 (2)	0.067 (3)	0.047 (2)	−0.039 (2)	0.0079 (19)	−0.011 (2)
C18	0.060 (3)	0.091 (4)	0.056 (3)	−0.052 (3)	0.005 (2)	−0.013 (3)
C19	0.043 (2)	0.109 (4)	0.048 (3)	−0.043 (3)	−0.002 (2)	−0.016 (3)
C110	0.033 (2)	0.094 (3)	0.040 (2)	−0.031 (2)	−0.0004 (17)	−0.018 (2)
C10A	0.0320 (19)	0.067 (3)	0.032 (2)	−0.0229 (18)	−0.0003 (16)	−0.0126 (18)
C111	0.0316 (19)	0.062 (3)	0.038 (2)	−0.0177 (18)	−0.0115 (17)	−0.0019 (19)
O111	0.0427 (16)	0.089 (2)	0.0652 (19)	−0.0270 (15)	−0.0303 (15)	0.0256 (17)
C11A	0.0286 (17)	0.040 (2)	0.0308 (18)	−0.0138 (15)	−0.0075 (15)	−0.0029 (15)
N112	0.0269 (15)	0.0425 (17)	0.0391 (17)	−0.0139 (13)	−0.0185 (13)	0.0091 (13)
C12A	0.0258 (16)	0.0290 (18)	0.0303 (18)	−0.0099 (13)	−0.0086 (14)	−0.0004 (14)
S12	0.0474 (5)	0.0317 (5)	0.0365 (5)	−0.0197 (4)	−0.0137 (4)	0.0068 (4)
C121	0.084 (3)	0.047 (3)	0.059 (3)	−0.028 (2)	−0.037 (2)	0.024 (2)
C151	0.0286 (17)	0.0314 (18)	0.0311 (18)	−0.0156 (14)	−0.0154 (14)	0.0064 (14)
C152	0.042 (2)	0.0239 (18)	0.036 (2)	−0.0092 (15)	−0.0129 (16)	0.0037 (15)
C153	0.042 (2)	0.036 (2)	0.034 (2)	−0.0143 (16)	−0.0108 (16)	0.0085 (16)
C154	0.0348 (18)	0.0289 (19)	0.037 (2)	−0.0076 (15)	−0.0130 (16)	0.0025 (15)
C155	0.055 (2)	0.0287 (19)	0.041 (2)	−0.0143 (17)	−0.0143 (19)	0.0074 (17)
C156	0.050 (2)	0.034 (2)	0.0317 (19)	−0.0157 (17)	−0.0125 (17)	0.0078 (16)
O154	0.0543 (16)	0.0324 (14)	0.0371 (14)	−0.0064 (12)	−0.0097 (12)	0.0042 (11)
C158	0.062 (3)	0.043 (2)	0.039 (2)	−0.002 (2)	−0.004 (2)	0.0052 (18)
N21	0.0240 (14)	0.0307 (15)	0.0327 (15)	−0.0040 (11)	−0.0109 (12)	0.0007 (12)
C22	0.0248 (16)	0.0312 (18)	0.0299 (18)	−0.0075 (13)	−0.0079 (14)	0.0064 (14)
N23	0.0188 (13)	0.0329 (15)	0.0327 (15)	−0.0059 (11)	−0.0118 (12)	0.0035 (12)
C24	0.0216 (16)	0.0278 (17)	0.0283 (17)	−0.0078 (13)	−0.0073 (13)	0.0068 (14)
O24	0.0272 (12)	0.0323 (13)	0.0364 (13)	−0.0066 (10)	−0.0151 (10)	0.0004 (10)
C24A	0.0242 (16)	0.0263 (17)	0.0273 (17)	−0.0089 (13)	−0.0090 (13)	0.0067 (13)
C25	0.0237 (16)	0.0310 (18)	0.0270 (17)	−0.0073 (13)	−0.0102 (13)	0.0017 (14)
C25A	0.0203 (15)	0.0303 (18)	0.0298 (17)	−0.0062 (13)	−0.0090 (13)	0.0084 (14)
C26	0.0296 (17)	0.0266 (18)	0.0318 (18)	−0.0108 (14)	−0.0066 (15)	0.0058 (15)
O26	0.0324 (13)	0.0393 (14)	0.0452 (15)	−0.0079 (11)	−0.0038 (11)	−0.0065 (12)

C26A	0.0207 (16)	0.0326 (18)	0.0331 (18)	−0.0052 (13)	−0.0040 (14)	0.0108 (15)
C27	0.0317 (19)	0.037 (2)	0.042 (2)	−0.0090 (16)	−0.0025 (16)	0.0086 (16)
C28	0.0223 (18)	0.047 (2)	0.057 (3)	−0.0021 (16)	−0.0017 (17)	0.013 (2)
C29	0.0232 (18)	0.052 (2)	0.046 (2)	−0.0100 (16)	−0.0078 (16)	0.0157 (19)
C210	0.0243 (17)	0.049 (2)	0.0338 (19)	−0.0110 (16)	−0.0080 (15)	0.0115 (16)
C20A	0.0246 (17)	0.039 (2)	0.0301 (18)	−0.0119 (14)	−0.0079 (14)	0.0128 (15)
C211	0.0245 (17)	0.038 (2)	0.0334 (19)	−0.0120 (14)	−0.0093 (15)	0.0080 (16)
O211	0.0306 (13)	0.0600 (17)	0.0548 (17)	−0.0158 (12)	−0.0128 (12)	−0.0160 (14)
C21A	0.0237 (16)	0.0312 (18)	0.0269 (17)	−0.0111 (14)	−0.0063 (14)	0.0064 (14)
N212	0.0208 (13)	0.0305 (15)	0.0319 (15)	−0.0055 (11)	−0.0107 (12)	−0.0032 (12)
C22A	0.0259 (16)	0.0292 (17)	0.0264 (17)	−0.0096 (14)	−0.0106 (14)	0.0082 (14)
S22	0.0296 (5)	0.0461 (6)	0.0411 (5)	0.0028 (4)	−0.0082 (4)	−0.0039 (4)
C221	0.056 (3)	0.060 (3)	0.059 (3)	0.007 (2)	−0.017 (2)	−0.023 (2)
C251	0.0181 (15)	0.0305 (18)	0.0339 (18)	−0.0074 (13)	−0.0103 (14)	0.0034 (14)
C252	0.0378 (19)	0.0298 (18)	0.0342 (19)	−0.0118 (15)	−0.0152 (16)	0.0012 (15)
C253	0.042 (2)	0.044 (2)	0.0263 (18)	−0.0172 (17)	−0.0114 (16)	0.0034 (16)
C254	0.0322 (18)	0.037 (2)	0.041 (2)	−0.0126 (15)	−0.0100 (16)	0.0081 (16)
C255	0.042 (2)	0.0304 (19)	0.037 (2)	−0.0111 (16)	−0.0047 (16)	−0.0058 (15)
C256	0.0317 (18)	0.0340 (19)	0.0350 (19)	−0.0111 (15)	−0.0046 (15)	−0.0008 (15)
O254	0.0709 (19)	0.0439 (16)	0.0405 (15)	−0.0301 (14)	−0.0065 (14)	0.0066 (12)
C258	0.126 (5)	0.076 (3)	0.041 (3)	−0.067 (3)	−0.004 (3)	0.008 (2)
N31	0.0264 (14)	0.0330 (15)	0.0304 (15)	−0.0128 (12)	−0.0132 (12)	0.0054 (12)
C32	0.0232 (16)	0.0285 (17)	0.0281 (17)	−0.0092 (13)	−0.0047 (13)	0.0009 (14)
N33	0.0202 (13)	0.0334 (15)	0.0336 (15)	−0.0118 (11)	−0.0111 (12)	0.0054 (12)
C34	0.0237 (16)	0.0323 (18)	0.0323 (18)	−0.0119 (14)	−0.0082 (14)	0.0036 (15)
O34	0.0310 (12)	0.0366 (13)	0.0415 (14)	−0.0153 (10)	−0.0210 (11)	0.0138 (11)
C34A	0.0243 (16)	0.0329 (18)	0.0325 (18)	−0.0141 (14)	−0.0088 (14)	0.0052 (14)
C35	0.0266 (17)	0.038 (2)	0.0358 (19)	−0.0164 (15)	−0.0147 (15)	0.0123 (15)
C35A	0.0259 (17)	0.040 (2)	0.0338 (19)	−0.0138 (15)	−0.0090 (15)	0.0043 (15)
C36	0.0250 (17)	0.041 (2)	0.0351 (19)	−0.0154 (15)	−0.0055 (15)	0.0074 (16)
O36	0.0367 (14)	0.0584 (17)	0.0549 (16)	−0.0278 (12)	−0.0215 (13)	0.0290 (14)
C36A	0.0228 (16)	0.042 (2)	0.0297 (18)	−0.0154 (14)	−0.0031 (14)	0.0029 (15)
C37	0.0296 (18)	0.046 (2)	0.047 (2)	−0.0215 (16)	−0.0084 (16)	0.0093 (17)
C38	0.0361 (19)	0.052 (2)	0.041 (2)	−0.0289 (17)	−0.0089 (17)	0.0024 (18)
C39	0.0247 (17)	0.055 (2)	0.0343 (19)	−0.0214 (16)	−0.0046 (15)	−0.0067 (17)
C310	0.0258 (17)	0.049 (2)	0.0276 (18)	−0.0144 (15)	−0.0041 (14)	−0.0024 (15)
C30A	0.0212 (16)	0.041 (2)	0.0274 (17)	−0.0138 (14)	−0.0027 (14)	−0.0008 (15)
C311	0.0251 (17)	0.044 (2)	0.0283 (18)	−0.0134 (15)	−0.0086 (14)	0.0036 (16)
O311	0.0330 (13)	0.0479 (15)	0.0517 (16)	−0.0167 (11)	−0.0221 (12)	0.0179 (13)
C31A	0.0217 (16)	0.0350 (19)	0.0278 (17)	−0.0126 (14)	−0.0066 (13)	0.0012 (14)
N312	0.0251 (14)	0.0364 (16)	0.0343 (16)	−0.0159 (12)	−0.0161 (12)	0.0117 (12)
C32A	0.0228 (16)	0.0338 (18)	0.0304 (18)	−0.0137 (14)	−0.0093 (14)	0.0020 (14)
S32	0.0300 (4)	0.0324 (5)	0.0372 (5)	−0.0160 (4)	−0.0124 (4)	0.0068 (4)
C321	0.042 (2)	0.035 (2)	0.056 (2)	−0.0164 (16)	−0.0226 (19)	0.0161 (18)
C351	0.0275 (17)	0.0368 (19)	0.037 (2)	−0.0219 (15)	−0.0151 (15)	0.0125 (15)
C352	0.0332 (18)	0.0340 (19)	0.038 (2)	−0.0177 (16)	−0.0152 (16)	0.0158 (16)
C353	0.040 (2)	0.049 (2)	0.0285 (18)	−0.0258 (18)	−0.0154 (16)	0.0088 (16)
C354	0.0297 (18)	0.0325 (19)	0.041 (2)	−0.0178 (15)	−0.0085 (16)	0.0025 (16)
C355	0.0301 (18)	0.040 (2)	0.037 (2)	−0.0201 (16)	−0.0182 (16)	0.0143 (16)

C356	0.0323 (18)	0.037 (2)	0.0366 (19)	−0.0190 (16)	−0.0143 (16)	0.0103 (16)
O354	0.0424 (14)	0.0459 (15)	0.0402 (14)	−0.0206 (12)	−0.0169 (12)	0.0095 (12)
C358	0.039 (2)	0.047 (2)	0.050 (2)	−0.0181 (17)	−0.0135 (18)	0.0018 (18)

Geometric parameters (Å, º)

N11—C12	1.318 (4)	C210—H210	0.9500
N11—C12A	1.371 (4)	C20A—C211	1.480 (5)
C12—N13	1.350 (4)	C211—O211	1.217 (4)
C12—S12	1.750 (3)	C211—C21A	1.493 (4)
N13—C14	1.383 (4)	C21A—N212	1.373 (4)
N13—H13	0.9170	N212—C22A	1.389 (4)
C14—O14	1.243 (3)	N212—H212	0.9799
C14—C14A	1.422 (4)	S22—C221	1.791 (4)
C14A—C12A	1.372 (4)	C221—H22A	0.9800
C14A—C15	1.512 (4)	C221—H22B	0.9800
C15—C15A	1.517 (4)	C221—H22C	0.9800
C15—C151	1.523 (5)	C251—C256	1.386 (5)
C15—H15	1.0000	C251—C252	1.393 (5)
C15A—C11A	1.360 (5)	C252—C253	1.382 (5)
C15A—C16	1.466 (5)	C252—H252	0.9500
C16—O16	1.233 (4)	C253—C254	1.375 (5)
C16—C16A	1.489 (5)	C253—H253	0.9500
C16A—C17	1.391 (5)	C254—O254	1.373 (4)
C16A—C10A	1.401 (5)	C254—C255	1.386 (5)
C17—C18	1.411 (6)	C255—C256	1.385 (5)
C17—H17	0.9500	C255—H255	0.9500
C18—C19	1.374 (7)	C256—H256	0.9500
C18—H18	0.9500	O254—C258	1.426 (5)
C19—C110	1.381 (6)	C258—H28A	0.9800
C19—H19	0.9500	C258—H28B	0.9800
C110—C10A	1.401 (5)	C258—H28C	0.9800
C110—H110	0.9500	N31—C32	1.310 (4)
C10A—C111	1.472 (5)	N31—C32A	1.368 (4)
C111—O111	1.232 (4)	C32—N33	1.357 (4)
C111—C11A	1.489 (4)	C32—S32	1.746 (3)
C11A—N112	1.380 (4)	N33—C34	1.387 (4)
N112—C12A	1.381 (4)	N33—H33	0.8750
N112—H112	0.9537	C34—O34	1.241 (4)
S12—C121	1.793 (4)	C34—C34A	1.431 (4)
C121—H12A	0.9800	C34A—C32A	1.370 (4)
C121—H12B	0.9800	C34A—C35	1.517 (4)
C121—H12C	0.9800	C35—C35A	1.524 (4)
C151—C152	1.378 (5)	C35—C351	1.536 (5)
C151—C156	1.406 (5)	C35—H35	1.0000
C152—C153	1.390 (5)	C35A—C31A	1.343 (4)
C152—H152	0.9500	C35A—C36	1.469 (4)
C153—C154	1.373 (5)	C36—O36	1.222 (4)
C153—H153	0.9500	C36—C36A	1.503 (4)
C154—O154	1.371 (4)	C36A—C37	1.389 (4)

C154—C155	1.391 (5)	C36A—C30A	1.391 (4)
C155—C156	1.374 (5)	C37—C38	1.384 (4)
C155—H155	0.9500	C37—H37	0.9500
C156—H156	0.9500	C38—C39	1.385 (5)
O154—C158	1.423 (4)	C38—H38	0.9500
C158—H18A	0.9800	C39—C310	1.380 (5)
C158—H18B	0.9800	C39—H39	0.9500
C158—H18C	0.9800	C310—C30A	1.400 (4)
N21—C22	1.313 (4)	C310—H310	0.9500
N21—C22A	1.370 (4)	C30A—C311	1.479 (4)
C22—N23	1.361 (4)	C311—O311	1.223 (4)
C22—S22	1.735 (3)	C311—C31A	1.504 (4)
N23—C24	1.383 (4)	C31A—N312	1.369 (4)
N23—H23	0.9322	N312—C32A	1.381 (4)
C24—O24	1.238 (4)	N312—H312	1.0027
C24—C24A	1.437 (4)	S32—C321	1.791 (3)
C24A—C22A	1.367 (4)	C321—H32A	0.9800
C24A—C25	1.499 (4)	C321—H32B	0.9800
C25—C25A	1.519 (4)	C321—H32C	0.9800
C25—C251	1.530 (4)	C351—C352	1.379 (5)
C25—H25	1.0000	C351—C356	1.393 (4)
C25A—C21A	1.356 (4)	C352—C353	1.370 (5)
C25A—C26	1.455 (4)	C352—H352	0.9500
C26—O26	1.222 (4)	C353—C354	1.404 (5)
C26—C26A	1.497 (4)	C353—H353	0.9500
C26A—C20A	1.389 (5)	C354—O354	1.367 (4)
C26A—C27	1.390 (5)	C354—C355	1.381 (5)
C27—C28	1.397 (5)	C355—C356	1.384 (5)
C27—H27	0.9500	C355—H355	0.9500
C28—C29	1.378 (5)	C356—H356	0.9500
C28—H28	0.9500	O354—C358	1.444 (4)
C29—C210	1.373 (5)	C358—H38A	0.9800
C29—H29	0.9500	C358—H38B	0.9800
C210—C20A	1.407 (4)	C358—H38C	0.9800

C12—N11—C12A	115.0 (3)	O211—C211—C21A	119.5 (3)
N11—C12—N13	123.6 (3)	C20A—C211—C21A	117.5 (3)
N11—C12—S12	122.2 (2)	C25A—C21A—N212	122.4 (3)
N13—C12—S12	114.3 (2)	C25A—C21A—C211	122.1 (3)
C12—N13—C14	122.9 (2)	N212—C21A—C211	115.4 (3)
C12—N13—H13	122.7	C21A—N212—C22A	120.6 (3)
C14—N13—H13	114.0	C21A—N212—H212	122.6
O14—C14—N13	120.8 (3)	C22A—N212—H212	116.8
O14—C14—C14A	123.9 (3)	C24A—C22A—N21	125.6 (3)
N13—C14—C14A	115.2 (3)	C24A—C22A—N212	119.6 (3)
C12A—C14A—C14	117.5 (3)	N21—C22A—N212	114.8 (3)
C12A—C14A—C15	122.3 (3)	C22—S22—C221	101.05 (17)
C14—C14A—C15	119.7 (3)	S22—C221—H22A	109.5
C14A—C15—C15A	109.0 (3)	S22—C221—H22B	109.5

C14A—C15—C151	111.5 (3)	H22A—C221—H22B	109.5
C15A—C15—C151	108.4 (2)	S22—C221—H22C	109.5
C14A—C15—H15	109.3	H22A—C221—H22C	109.5
C15A—C15—H15	109.3	H22B—C221—H22C	109.5
C151—C15—H15	109.3	C256—C251—C252	117.7 (3)
C11A—C15A—C16	120.2 (3)	C256—C251—C25	122.0 (3)
C11A—C15A—C15	120.6 (3)	C252—C251—C25	120.2 (3)
C16—C15A—C15	119.1 (3)	C253—C252—C251	122.1 (3)
O16—C16—C15A	120.9 (3)	C253—C252—H252	118.9
O16—C16—C16A	120.9 (3)	C251—C252—H252	118.9
C15A—C16—C16A	118.3 (3)	C254—C253—C252	119.0 (3)
C17—C16A—C10A	120.5 (3)	C254—C253—H253	120.5
C17—C16A—C16	119.0 (4)	C252—C253—H253	120.5
C10A—C16A—C16	120.5 (3)	O254—C254—C253	124.0 (3)
C16A—C17—C18	118.0 (4)	O254—C254—C255	115.7 (3)
C16A—C17—H17	121.0	C253—C254—C255	120.3 (3)
C18—C17—H17	121.0	C256—C255—C254	120.0 (3)
C19—C18—C17	121.5 (4)	C256—C255—H255	120.0
C19—C18—H18	119.2	C254—C255—H255	120.0
C17—C18—H18	119.2	C255—C256—C251	120.8 (3)
C18—C19—C110	120.5 (4)	C255—C256—H256	119.6
C18—C19—H19	119.8	C251—C256—H256	119.6
C110—C19—H19	119.8	C254—O254—C258	117.0 (3)
C19—C110—C10A	119.3 (4)	O254—C258—H28A	109.5
C19—C110—H110	120.4	O254—C258—H28B	109.5
C10A—C110—H110	120.4	H28A—C258—H28B	109.5
C16A—C10A—C110	120.2 (4)	O254—C258—H28C	109.5
C16A—C10A—C111	120.1 (3)	H28A—C258—H28C	109.5
C110—C10A—C111	119.7 (4)	H28B—C258—H28C	109.5
O111—C111—C10A	123.3 (3)	C32—N31—C32A	115.2 (3)
O111—C111—C11A	119.0 (3)	N31—C32—N33	123.4 (3)
C10A—C111—C11A	117.7 (3)	N31—C32—S32	122.6 (2)
C15A—C11A—N112	122.1 (3)	N33—C32—S32	114.0 (2)
C15A—C11A—C111	122.4 (3)	C32—N33—C34	123.1 (2)
N112—C11A—C111	115.5 (3)	C32—N33—H33	121.3
C11A—N112—C12A	120.6 (3)	C34—N33—H33	115.0
C11A—N112—H112	123.5	O34—C34—N33	120.0 (3)
C12A—N112—H112	115.9	O34—C34—C34A	125.2 (3)
N11—C12A—C14A	125.5 (3)	N33—C34—C34A	114.8 (3)
N11—C12A—N112	114.9 (3)	C32A—C34A—C34	117.2 (3)
C14A—C12A—N112	119.6 (3)	C32A—C34A—C35	124.0 (3)
C12—S12—C121	102.29 (17)	C34—C34A—C35	118.8 (3)
S12—C121—H12A	109.5	C34A—C35—C35A	109.0 (3)
S12—C121—H12B	109.5	C34A—C35—C351	111.2 (3)
H12A—C121—H12B	109.5	C35A—C35—C351	110.7 (3)
S12—C121—H12C	109.5	C34A—C35—H35	108.6
H12A—C121—H12C	109.5	C35A—C35—H35	108.6
H12B—C121—H12C	109.5	C351—C35—H35	108.6
C152—C151—C156	116.6 (3)	C31A—C35A—C36	120.4 (3)

C152—C151—C15	122.3 (3)	C31A—C35A—C35	122.1 (3)
C156—C151—C15	120.9 (3)	C36—C35A—C35	117.4 (3)
C151—C152—C153	122.4 (3)	O36—C36—C35A	120.9 (3)
C151—C152—H152	118.8	O36—C36—C36A	121.3 (3)
C153—C152—H152	118.8	C35A—C36—C36A	117.7 (3)
C154—C153—C152	119.7 (3)	C37—C36A—C30A	119.4 (3)
C154—C153—H153	120.2	C37—C36A—C36	119.0 (3)
C152—C153—H153	120.2	C30A—C36A—C36	121.5 (3)
O154—C154—C153	124.5 (3)	C38—C37—C36A	119.9 (3)
O154—C154—C155	116.0 (3)	C38—C37—H37	120.0
C153—C154—C155	119.5 (3)	C36A—C37—H37	120.0
C156—C155—C154	120.0 (3)	C37—C38—C39	120.7 (3)
C156—C155—H155	120.0	C37—C38—H38	119.7
C154—C155—H155	120.0	C39—C38—H38	119.7
C155—C156—C151	121.7 (3)	C310—C39—C38	120.1 (3)
C155—C156—H156	119.2	C310—C39—H39	120.0
C151—C156—H156	119.2	C38—C39—H39	120.0
C154—O154—C158	116.7 (3)	C39—C310—C30A	119.5 (3)
O154—C158—H18A	109.5	C39—C310—H310	120.3
O154—C158—H18B	109.5	C30A—C310—H310	120.3
H18A—C158—H18B	109.5	C36A—C30A—C310	120.4 (3)
O154—C158—H18C	109.5	C36A—C30A—C311	119.8 (3)
H18A—C158—H18C	109.5	C310—C30A—C311	119.8 (3)
H18B—C158—H18C	109.5	O311—C311—C30A	123.9 (3)
C22—N21—C22A	115.4 (3)	O311—C311—C31A	119.1 (3)
N21—C22—N23	123.6 (3)	C30A—C311—C31A	117.0 (3)
N21—C22—S22	122.3 (3)	C35A—C31A—N312	123.2 (3)
N23—C22—S22	114.1 (2)	C35A—C31A—C311	123.3 (3)
C22—N23—C24	122.7 (2)	N312—C31A—C311	113.4 (3)
C22—N23—H23	121.6	C31A—N312—C32A	120.6 (3)
C24—N23—H23	115.6	C31A—N312—H312	118.6
O24—C24—N23	121.0 (3)	C32A—N312—H312	120.7
O24—C24—C24A	124.1 (3)	N31—C32A—C34A	126.1 (3)
N23—C24—C24A	114.9 (3)	N31—C32A—N312	114.2 (3)
C22A—C24A—C24	117.7 (3)	C34A—C32A—N312	119.7 (3)
C22A—C24A—C25	123.2 (3)	C32—S32—C321	101.51 (15)
C24—C24A—C25	118.7 (3)	S32—C321—H32A	109.5
C24A—C25—C25A	109.6 (3)	S32—C321—H32B	109.5
C24A—C25—C251	109.1 (3)	H32A—C321—H32B	109.5
C25A—C25—C251	110.3 (2)	S32—C321—H32C	109.5
C24A—C25—H25	109.3	H32A—C321—H32C	109.5
C25A—C25—H25	109.3	H32B—C321—H32C	109.5
C251—C25—H25	109.3	C352—C351—C356	117.8 (3)
C21A—C25A—C26	120.7 (3)	C352—C351—C35	120.2 (3)
C21A—C25A—C25	121.2 (3)	C356—C351—C35	121.9 (3)
C26—C25A—C25	118.1 (3)	C353—C352—C351	121.9 (3)
O26—C26—C25A	120.8 (3)	C353—C352—H352	119.1
O26—C26—C26A	120.5 (3)	C351—C352—H352	119.1
C25A—C26—C26A	118.7 (3)	C352—C353—C354	119.9 (3)

C20A—C26A—C27	119.9 (3)	C352—C353—H353	120.0
C20A—C26A—C26	120.4 (3)	C354—C353—H353	120.0
C27—C26A—C26	119.7 (3)	O354—C354—C355	124.5 (3)
C26A—C27—C28	119.4 (4)	O354—C354—C353	116.4 (3)
C26A—C27—H27	120.3	C355—C354—C353	119.1 (3)
C28—C27—H27	120.3	C354—C355—C356	119.9 (3)
C29—C28—C27	120.5 (3)	C354—C355—H355	120.1
C29—C28—H28	119.8	C356—C355—H355	120.1
C27—C28—H28	119.8	C355—C356—C351	121.4 (3)
C210—C29—C28	120.7 (3)	C355—C356—H356	119.3
C210—C29—H29	119.7	C351—C356—H356	119.3
C28—C29—H29	119.7	C354—O354—C358	117.9 (3)
C29—C210—C20A	119.5 (4)	O354—C358—H38A	109.5
C29—C210—H210	120.3	O354—C358—H38B	109.5
C20A—C210—H210	120.3	H38A—C358—H38B	109.5
C26A—C20A—C210	120.1 (3)	O354—C358—H38C	109.5
C26A—C20A—C211	120.3 (3)	H38A—C358—H38C	109.5
C210—C20A—C211	119.6 (3)	H38B—C358—H38C	109.5
O211—C211—C20A	122.9 (3)		

C12A—N11—C12—N13	−2.5 (5)	C26A—C20A—C211—C21A	2.1 (4)
C12A—N11—C12—S12	177.9 (2)	C210—C20A—C211—C21A	−177.4 (3)
N11—C12—N13—C14	4.8 (5)	C26—C25A—C21A—N212	177.4 (3)
S12—C12—N13—C14	−175.5 (2)	C25—C25A—C21A—N212	−5.2 (5)
C12—N13—C14—O14	177.4 (3)	C26—C25A—C21A—C211	−5.7 (5)
C12—N13—C14—C14A	−2.0 (4)	C25—C25A—C21A—C211	171.7 (3)
O14—C14—C14A—C12A	178.1 (3)	O211—C211—C21A—C25A	−176.1 (3)
N13—C14—C14A—C12A	−2.5 (4)	C20A—C211—C21A—C25A	0.9 (4)
O14—C14—C14A—C15	−10.1 (5)	O211—C211—C21A—N212	1.0 (4)
N13—C14—C14A—C15	169.3 (3)	C20A—C211—C21A—N212	178.0 (3)
C12A—C14A—C15—C15A	−26.1 (4)	C25A—C21A—N212—C22A	−6.8 (4)
C14—C14A—C15—C15A	162.4 (3)	C211—C21A—N212—C22A	176.1 (3)
C12A—C14A—C15—C151	93.6 (4)	C24—C24A—C22A—N21	4.4 (5)
C14—C14A—C15—C151	−77.9 (4)	C25—C24A—C22A—N21	−167.7 (3)
C14A—C15—C15A—C11A	23.6 (4)	C24—C24A—C22A—N212	−176.3 (3)
C151—C15—C15A—C11A	−98.0 (4)	C25—C24A—C22A—N212	11.5 (4)
C14A—C15—C15A—C16	−161.2 (3)	C22—N21—C22A—C24A	−1.6 (4)
C151—C15—C15A—C16	77.2 (4)	C22—N21—C22A—N212	179.1 (3)
C11A—C15A—C16—O16	−170.7 (3)	C21A—N212—C22A—C24A	3.7 (4)
C15—C15A—C16—O16	14.1 (5)	C21A—N212—C22A—N21	−176.9 (3)
C11A—C15A—C16—C16A	10.9 (5)	N21—C22—S22—C221	3.1 (3)
C15—C15A—C16—C16A	−164.3 (3)	N23—C22—S22—C221	−176.4 (3)
O16—C16—C16A—C17	−9.0 (5)	C24A—C25—C251—C256	130.8 (3)
C15A—C16—C16A—C17	169.4 (3)	C25A—C25—C251—C256	−108.8 (3)
O16—C16—C16A—C10A	170.9 (3)	C24A—C25—C251—C252	−48.0 (4)
C15A—C16—C16A—C10A	−10.8 (5)	C25A—C25—C251—C252	72.4 (4)
C10A—C16A—C17—C18	0.2 (6)	C256—C251—C252—C253	−1.7 (5)
C16—C16A—C17—C18	−180.0 (3)	C25—C251—C252—C253	177.1 (3)
C16A—C17—C18—C19	−1.6 (6)	C251—C252—C253—C254	−0.2 (5)

C17—C18—C19—C110	1.2 (7)	C252—C253—C254—O254	−177.6 (3)
C18—C19—C110—C10A	0.6 (6)	C252—C253—C254—C255	1.4 (5)
C17—C16A—C10A—C110	1.6 (6)	O254—C254—C255—C256	178.4 (3)
C16—C16A—C10A—C110	−178.3 (3)	C253—C254—C255—C256	−0.6 (5)
C17—C16A—C10A—C111	−176.3 (3)	C254—C255—C256—C251	−1.3 (5)
C16—C16A—C10A—C111	3.9 (5)	C252—C251—C256—C255	2.4 (5)
C19—C110—C10A—C16A	−2.0 (6)	C25—C251—C256—C255	−176.4 (3)
C19—C110—C10A—C111	175.9 (4)	C253—C254—O254—C258	−6.1 (5)
C16A—C10A—C111—O111	179.1 (4)	C255—C254—O254—C258	174.9 (4)
C110—C10A—C111—O111	1.2 (6)	C32A—N31—C32—N33	1.5 (5)
C16A—C10A—C111—C11A	2.9 (5)	C32A—N31—C32—S32	−178.9 (2)
C110—C10A—C111—C11A	−175.0 (3)	N31—C32—N33—C34	−0.7 (5)
C16—C15A—C11A—N112	177.2 (3)	S32—C32—N33—C34	179.7 (2)
C15—C15A—C11A—N112	−7.7 (5)	C32—N33—C34—O34	176.3 (3)
C16—C15A—C11A—C111	−4.3 (5)	C32—N33—C34—C34A	−2.4 (5)
C15—C15A—C11A—C111	170.8 (3)	O34—C34—C34A—C32A	−174.1 (3)
O111—C111—C11A—C15A	−179.1 (4)	N33—C34—C34A—C32A	4.6 (5)
C10A—C111—C11A—C15A	−2.7 (5)	O34—C34—C34A—C35	6.7 (5)
O111—C111—C11A—N112	−0.5 (5)	N33—C34—C34A—C35	−174.7 (3)
C10A—C111—C11A—N112	175.9 (3)	C32A—C34A—C35—C35A	12.7 (5)
C15A—C11A—N112—C12A	−9.8 (5)	C34—C34A—C35—C35A	−168.1 (3)
C111—C11A—N112—C12A	171.6 (3)	C32A—C34A—C35—C351	−109.7 (4)
C12—N11—C12A—C14A	−2.5 (5)	C34—C34A—C35—C351	69.5 (4)
C12—N11—C12A—N112	178.8 (3)	C34A—C35—C35A—C31A	−10.8 (5)
C14—C14A—C12A—N11	5.0 (5)	C351—C35—C35A—C31A	111.8 (4)
C15—C14A—C12A—N11	−166.6 (3)	C34A—C35—C35A—C36	172.3 (3)
C14—C14A—C12A—N112	−176.4 (3)	C351—C35—C35A—C36	−65.1 (4)
C15—C14A—C12A—N112	12.0 (5)	C31A—C35A—C36—O36	174.9 (3)
C11A—N112—C12A—N11	−173.7 (3)	C35—C35A—C36—O36	−8.1 (5)
C11A—N112—C12A—C14A	7.6 (5)	C31A—C35A—C36—C36A	−5.5 (5)
N11—C12—S12—C121	−16.4 (3)	C35—C35A—C36—C36A	171.4 (3)
N13—C12—S12—C121	163.9 (3)	O36—C36—C36A—C37	6.3 (5)
C14A—C15—C151—C152	−25.5 (4)	C35A—C36—C36A—C37	−173.2 (3)
C15A—C15—C151—C152	94.5 (3)	O36—C36—C36A—C30A	−174.7 (3)
C14A—C15—C151—C156	159.7 (3)	C35A—C36—C36A—C30A	5.7 (5)
C15A—C15—C151—C156	−80.2 (3)	C30A—C36A—C37—C38	1.0 (5)
C156—C151—C152—C153	0.6 (5)	C36—C36A—C37—C38	180.0 (3)
C15—C151—C152—C153	−174.3 (3)	C36A—C37—C38—C39	0.4 (6)
C151—C152—C153—C154	0.3 (5)	C37—C38—C39—C310	−0.5 (6)
C152—C153—C154—O154	177.4 (3)	C38—C39—C310—C30A	−0.7 (5)
C152—C153—C154—C155	−1.5 (5)	C37—C36A—C30A—C310	−2.2 (5)
O154—C154—C155—C156	−177.2 (3)	C36—C36A—C30A—C310	178.8 (3)
C153—C154—C155—C156	1.8 (5)	C37—C36A—C30A—C311	176.5 (3)
C154—C155—C156—C151	−1.0 (5)	C36—C36A—C30A—C311	−2.5 (5)
C152—C151—C156—C155	−0.2 (5)	C39—C310—C30A—C36A	2.1 (5)
C15—C151—C156—C155	174.8 (3)	C39—C310—C30A—C311	−176.6 (3)
C153—C154—O154—C158	−12.7 (5)	C36A—C30A—C311—O311	−178.4 (3)
C155—C154—O154—C158	166.3 (3)	C310—C30A—C311—O311	0.3 (5)
C22A—N21—C22—N23	−2.5 (4)	C36A—C30A—C311—C31A	−0.9 (5)

C22A—N21—C22—S22	178.0 (2)	C310—C30A—C311—C31A	177.8 (3)
N21—C22—N23—C24	3.6 (5)	C36—C35A—C31A—N312	179.5 (3)
S22—C22—N23—C24	−176.9 (2)	C35—C35A—C31A—N312	2.7 (5)
C22—N23—C24—O24	179.3 (3)	C36—C35A—C31A—C311	2.2 (5)
C22—N23—C24—C24A	−0.6 (4)	C35—C35A—C31A—C311	−174.6 (3)
O24—C24—C24A—C22A	177.0 (3)	O311—C311—C31A—C35A	178.7 (3)
N23—C24—C24A—C22A	−3.1 (4)	C30A—C311—C31A—C35A	1.1 (5)
O24—C24—C24A—C25	−10.5 (5)	O311—C311—C31A—N312	1.2 (5)
N23—C24—C24A—C25	169.4 (3)	C30A—C311—C31A—N312	−176.4 (3)
C22A—C24A—C25—C25A	−21.0 (4)	C35A—C31A—N312—C32A	5.7 (5)
C24—C24A—C25—C25A	167.0 (3)	C311—C31A—N312—C32A	−176.8 (3)
C22A—C24A—C25—C251	99.8 (3)	C32—N31—C32A—C34A	1.1 (5)
C24—C24A—C25—C251	−72.2 (3)	C32—N31—C32A—N312	−177.8 (3)
C24A—C25—C25A—C21A	17.6 (4)	C34—C34A—C32A—N31	−4.2 (5)
C251—C25—C25A—C21A	−102.5 (3)	C35—C34A—C32A—N31	174.9 (3)
C24A—C25—C25A—C26	−164.9 (3)	C34—C34A—C32A—N312	174.7 (3)
C251—C25—C25A—C26	75.0 (3)	C35—C34A—C32A—N312	−6.2 (5)
C21A—C25A—C26—O26	−173.3 (3)	C31A—N312—C32A—N31	175.1 (3)
C25—C25A—C26—O26	9.2 (4)	C31A—N312—C32A—C34A	−3.9 (5)
C21A—C25A—C26—C26A	7.3 (4)	N31—C32—S32—C321	−8.6 (3)
C25—C25A—C26—C26A	−170.2 (3)	N33—C32—S32—C321	171.1 (3)
O26—C26—C26A—C20A	176.3 (3)	C34A—C35—C351—C352	71.1 (3)
C25A—C26—C26A—C20A	−4.2 (4)	C35A—C35—C351—C352	−50.3 (4)
O26—C26—C26A—C27	−6.0 (5)	C34A—C35—C351—C356	−110.0 (3)
C25A—C26—C26A—C27	173.4 (3)	C35A—C35—C351—C356	128.7 (3)
C20A—C26A—C27—C28	−0.3 (5)	C356—C351—C352—C353	−0.1 (5)
C26—C26A—C27—C28	−178.0 (3)	C35—C351—C352—C353	178.9 (3)
C26A—C27—C28—C29	−0.6 (5)	C351—C352—C353—C354	−0.5 (5)
C27—C28—C29—C210	0.4 (5)	C352—C353—C354—O354	−178.6 (3)
C28—C29—C210—C20A	0.8 (5)	C352—C353—C354—C355	0.5 (5)
C27—C26A—C20A—C210	1.5 (5)	O354—C354—C355—C356	179.1 (3)
C26—C26A—C20A—C210	179.1 (3)	C353—C354—C355—C356	0.0 (4)
C27—C26A—C20A—C211	−178.0 (3)	C354—C355—C356—C351	−0.6 (5)
C26—C26A—C20A—C211	−0.4 (4)	C352—C351—C356—C355	0.7 (4)
C29—C210—C20A—C26A	−1.8 (5)	C35—C351—C356—C355	−178.3 (3)
C29—C210—C20A—C211	177.8 (3)	C355—C354—O354—C358	9.9 (4)
C26A—C20A—C211—O211	179.1 (3)	C353—C354—O354—C358	−171.0 (3)
C210—C20A—C211—O211	−0.5 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N13—H13···O34	0.92	1.84	2.757 (3)	173
N23—H23···O24^{i}	0.93	1.81	2.741 (3)	176
N33—H33···O14	0.87	1.86	2.702 (3)	160
N112—H112···N21	0.95	2.28	3.175 (4)	156
N212—H212···N11	0.98	2.21	3.125 (4)	154
N312—H312···O311	1.00	2.25	2.651 (4)	102
C255—H255···O26^{ii}	0.95	2.34	3.237 (4)	158

C352—H352···N31^{iii}	0.95	2.61	3.503 (4)	157
C29—H29···*Cg*^{iv}	0.95	2.79	3.659 (4)	152

Symmetry codes: (i) −*x*, −*y*+1, −*z*; (ii) −*x*+1, −*y*, −*z*; (iii) −*x*+2, −*y*+1, −*z*+1; (iv) *x*+1, *y*, *z*.

Selected geometric parameters (Å, °) for the R enantiomers of the three independent molecules in compound (I)

(*a*)	Torsion and bond angles		
	Molecule 1	Molecule 2	Molecule 3
	x = 1	*x* = 2	*x* = 3
N*x*1—C*x*2—S*x*2—C*x*21	-16.4 (3)	3.1 (3)	8.6 (3)
C*x*4*A*—C*x*5—C*x*51—C*x*52	-15.5 (4)	-48.0 (4)	-71.1 (3)
C*x*5*A*—C*x*5—C*x*51—C*x*52	94.5 (3)	72.4 (4)	50.3 (4)
C*x*53—C*x*54—O*x*54—C*x*58	-12.7 (5)	-6.1 (5)	171.0 (3)
N*x*1—C*x*2—S*x*2	122.2 (2)	122.3 (3)	122.6 (2)
N*x*3—C*x*2—S*x*2	114.3 (2)	114.1 (2)	114.0 (2)
C*x*53—C*x*54—O*x*54	124.5 (3)	124.0 (3)	116.4 (3)
C*x*55—C*x*54—O*x*54	116.0 (3)	115.7 (3)	124.5 (3)

(*b*)	Ring-puckering parameters		
	Molecule 1	Molecule 2	Molecule 3
Q	0.246 (4)	0.185 (4)	0.120 (4)
θ	111.4 (9)	113.8 (9)	109.5 (19)
φ	4.9 (9)	10.2 (12)	8.4 (19)

Ring-puckering angles are defined for the atom sequences N*x*12—C*x*1*A*—C*x*5*A*—C*x*5— C*x*4*A*—C*x*2*A* for *x* = 1, 2 or 3